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LETTER TO THE EDITOR

Renormalisation group recursions by mean-field approximations

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Abstract. Within a renormalisation group strategy, different 'rescaled' mean-field approximations for the magnetisation are combined. Good qualitative estimates are obtained for the critical properties of classical and quantum spin systems. A particularly simple realisation of the method yields recursions for arbitrary dimensionality d. The critical couplings are remarkably accurate for all d, and have the correct asymptotic behaviour for d approaching infinity.

In this Letter we present a new, efficient and easily applicable method for computing critical properties of lattice spin systems. Our approach is close in spirit to the so called 'phenomenological' renormalisation, based on the comparison of systems of different finite sizes (Nightingale 1976, 1977, Sneddon 1978). At the same time, our calculations are directly related to approximations of mean-field type for the equation of state. We show explicitly how a renormalisation strategy can improve on mean-field results, without involving further calculational effort. Some of the simplest realisations of our method also have a direct formal connection with more standard real-space renormalisation techniques (Niemeijer and van Leeuwen 1976) and we find it instructive to exploit this feature to introduce the general approach.

Let us consider, for simplicity, the case of a ferromagnetic Ising system on a d-dimensional hypercubic lattice.

The reduced Hamiltonian is

$$-\beta\mathcal{H}(s) = H(s) = K \sum_{\langle ij \rangle} s_i s_j + h \sum_i s_i \tag{1}$$

where $s_i = \pm 1$, $\beta = 1/k_B T$, K is the nearest-neighbour coupling and h the magnetic field.

By the standard machinery of real-space renormalisation, we can transform $H(s)$ into a renormalised $H'(s')$ appropriate to a system with spins s' on a lattice rescaled by a factor l with respect to the original one. One way of achieving this, with, for example, $l = 2$, consists in using a linear weight factor (Wilson 1975, Niemeijer and van Leeuwen 1976)

$$P(s', s) = \prod_\alpha \frac{1}{2}\left(1 + p\, s'_\alpha \sum_{i \in \alpha} s_i\right) \tag{2}$$

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where α runs over hypercubic cells of 2^d spins, into which we divide the lattice, and p is a parameter whose value is connected to the correlation function exponent η.

$H'(s')$ can be computed on the basis of a cumulant expansion in the inter-cell interactions (Niemeijer and van Leeuwen 1976). Up to first order in these interactions, $H'(s')$ stays of the form (1), with K' and h' parametrically dependent on p.

Linearising the transformation in h around $h=0$ and indicating $(\partial h'/\partial h)|_{h=0}$ by $\lambda_H(K)$, hyperscaling implies that at the fixed point K^* (Wilson 1975)

$$p\lambda_H(K^*)=1. \tag{3}$$

This suggests that p can be eliminated from the transformation by imposing (3) to hold identically for all K. One can see that the K dependence of p introduced in this way also guarantees the important property $\lambda_H \to 2^d$ for $K \to \infty$, which allows the existence of spontaneous magnetisation (Nienhuis and Nauenberg 1975). Computing K' and λ_H in the cumulant expansion up to first and zeroth orders, respectively, we obtain the transformation

$$K'=\tfrac{1}{2}Kf(K) \tag{4}$$

$$h'=\lambda_H(K)h=2^{d/2}f^{1/2}(K)h \tag{5}$$

with

$$f(K)=2^{-d}\left\langle\left(\sum_{i\in\alpha}s_i\right)^2\right\rangle_\alpha \tag{6}$$

where $\langle\ \rangle_\alpha$ is a zero-field cell average.

We now propose an alternative way of arriving at this result. The following derivation exemplifies the basic steps of our method. Let us consider two finite systems: a single spin and a hypercube with 2^d spins. For both systems we can compute the average magnetisation in the presence of symmetry-breaking boundary conditions, which, in a mean-field sense, simulate the effect of surrounding spins in infinite extensions of the systems. The single spin interacts with $2d$ nearest-neighbour spins fixed to a value b' ($|b'|\leqslant 1$), whereas each spin in the hypercube interacts with d boundary spins, whose value is b ($|b|\leqslant 1$). Let us indicate by f_1 (f_2) the function of the couplings and of b' (b), expressing the magnetisation per spin in the smaller (bigger) system. We can define a renormalisation mapping implicitly (in the neighbourhood of $h=0$) by imposing

$$f_1(K', h', b')=2^d p f_2(K, h, b) \tag{7}$$

and

$$b'=2^d pb \tag{8}$$

to leading orders in h and b, for b approaching zero.

Omitting the b' and b dependences and the subscripts, equation (7) would represent the transformation law for the magnetisation of the infinite system (to be indicated just by f) under the renormalisation mapping induced by (2). The quantities b and b' are related by the same law through (8), because they have the physical meaning of magnetisations. This meaning becomes clear by the observation that, for example, by equating f_1 to b' itself, we obtain the mean-field equation of state for the system. Replacing f_1 by f_2 and equating it to b, we also obtain an equation of state of the mean-field type, in which fluctuations within hypercubes of 2^d spins are taken into account.

One can now show that the recursions implied by (7) and (8) are precisely (4) and (5), by linearising in b, b' and h, putting $h' = \lambda_H h$ and assuming again that the hyperscaling relation (3) holds identically for all K. By imposing scaling requirements on approximations for the magnetisation, characterised by different 'typical lengths', we thus obtain in the above example the same results as by explicit elimination of degrees of freedom. The feature of working in the neighbourhood of b and b' equal to zero is appropriate to the study of second-order transitions. A generalisation of our methods to the description of first-order transitions should allow for finite b and b' values.

We have applied the simple scheme described above to $d = 1, 2$ and 3 Ising models. In one dimension we obtain only the $K^* = \infty$ and $K^* = 0$ fixed points, as we should†.

For $d = 2$ and 3 the results are reported in the rows of table 1 where $L = 2$ and $L' = 1$. These results indicate a rather satisfactory standard of qualitative accuracy in comparison with other real-space methods of similar complexity. It is also interesting to note the drastic improvement of our calculation with respect to the corresponding mean-field approximations. For example, in the case $d = 2$, the mean-field calculation gives $K_c = 0.250$, the improved one, using f_2, gives $K_c = 0.286$, whereas our result is much closer to the exact value.

Table 1. Results for the classical Ising model.

	L	L'	K_c	y_T	y_H
$d = 2$	2	1	0.361	0.69	1.50
	3	2	0.381	0.78	1.57
	4	3	0.393	0.82	1.60
	5	4	0.401	0.84	1.62
	Exact		0.441	1.000	1.875
$d = 3$	2	1	0.207	0.82	2.00
	3	2	0.212	0.95	2.08
			0.214[a]	1.587[b]	2.485[b]

[a] Domb (1974).
[b] Le Guillou and Zinn-Justin (1980).

The above presentation suggests very naturally how to generalise our recipe to systems of bigger sizes and hopefully improve the accuracy. Let us consider two finite hypercubic systems with $N' = L'^d$ and $N = L^d$ spins, respectively. We introduce symmetry-breaking boundary conditions as before and compute the average magnetisations per spin, indicated by $f_{L'}$ and f_L. In order to define the transformation, we impose (7) and (8), replacing 1 and 2 by L' and L, respectively, and 2^d by $(L/L')^d$. We remark that as soon as $L > 2$, the formal connection with cumulant approximations for linear transformations is lost, owing to the presence of non-equivalent spins in the cells and to the possibility of realising non-integer rescalings ($l = L/L'$). In the

† In this simple approximation, only the y_H exponent is given correctly at the $K^* = \infty$ fixed point in $d = 1$. In order to obtain also the exact y_T, one must perform a different calculation, involving the comparison of two chains with L and $L' = L - 1$ spins, respectively, in the limit $L \to \infty$.

general case, our scheme is equivalent to treating the inter-cell interactions in an effective-field approximation, within the framework of a linear renormalisation transformation. Non-integer rescalings can then be obtained by combining two transformations with integer rescalings.

In order to test the convergence of the method as the sizes of the systems increase, we performed calculations on a sequence of boxes with $L = 2, 3, 4$ and 5 in $d = 2$, and $L = 2$ and 3 in $d = 3$. As usual in calculations involving systems of finite sizes, the best results for a given L are obtained for $L' = L - 1$. These results are reported in table 1. Although the boxes considered are quite small, the results already show a definite, even if slow, convergence towards exact or expected results, especially for K_c. It would certainly be interesting to set up similar calculations on systems of bigger sizes, for example with the help of Monte Carlo or transfer matrix techniques. In this way, the efficiency of our method could be compared with that of finite-size scaling (Nightingale and Blöte 1980) or phenomenological renormalisation approaches (Nightingale 1976, 1977, Sneddon 1978).

We believe that among the most interesting features of our approach are its peculiar use of symmetry-breaking boundary conditions and its connection with approximations of mean-field type. These features allow the setting up in a very simple and direct way of recursion formulae where the dimensionality dependence is explicit, like in those of Migdal (1976), and K_c has the correct behaviour in the limit $d \to \infty$. The following most practical choice of systems is already sufficient for this purpose. The smaller one consists of the single spin system introduced before and the bigger one contains just two nearest-neighbour fluctuating spins, both surrounded by $(2d-1)$ fixed boundary spins (as illustrated schematically in figure 1 for $d = 3$). The rescaling factor

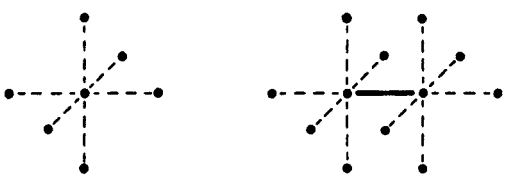

Figure 1. Schematic representation of the simplest choice of clusters for $d = 3$. Broken bonds represent interactions with boundary spins.

is now put equal to $2^{1/d}$. Working out this scheme for a q-state Potts model, with reduced Hamiltonian

$$H(s) = \frac{K}{q-1} \sum_{\langle ij \rangle} (q\delta_{s_i,s_j} - 1) + \frac{h}{q-1} \sum_i (q\delta_{s_i,0} - 1) \tag{9}$$

with $s_k = 0, 1, \ldots, q-1$, we find the following recursion for K:

$$K' = \frac{2d-1}{2d} K \left(1 + \frac{\exp[qK/(q-1)] - 1}{\exp[qK/(q-1)] - 1 + q}\right); \tag{10}$$

this leads to

$$K^* = K_c = \frac{q-1}{q} \ln\left(\frac{q + 2(d-1)}{2(d-1)}\right). \tag{11}$$

Equation (11) gives correctly $K_c \to \infty$ for $d \to 1$. Moreover, for $q = 2$ and $d \to \infty$

$$K_c = \frac{1}{2d} + \frac{1}{4d^2} + O\left(\frac{1}{d^3}\right), \tag{12}$$

which agrees, up to second order, with the exact $1/d$ expansion (Fisher and Gaunt 1964, Balian *et al* 1975). In this respect our transformation is superior to the well known Migdal (1976) recursion, which fails to give the correct asymptotic behaviour of K_c. The result (12) is a consequence of the relationship between our method and mean-field approximations, which become exact as $d \to \infty$. The values for K_c given by (11) are also in surprisingly good agreement with those obtained by other exact or approximate methods for $d = 2, 3$ and 4 and for general q. The discrepancies are always below 6% for $d \geqslant 3$. It is interesting to notice that, for $d = 2$ and $q = 4$, equation (11) yields the exact value for K_c (Baxter 1973). For $d = 3$ and $q = 3$, even if the actual transition is probably of first order, we obtain $K_c = 0.373$, which happens to be quite close to the value $K_c \simeq 0.367$ recently estimated by Monte Carlo methods (Blöte and Swendsen 1979) and $1/q$ expansion (Kogut and Sinclair 1981).

A mean-field approximation would give $K_c = 0.308$ in this case (Mittag and Stephen 1974). The improvement over mean-field values of K_c is also considerable at $d = 4$. In the Ising model ($q = 2$), for example, the mean-field approximation gives $K_c = 0.125$, which is poorer than our value $K_c = 0.144$ with respect to the value $K_c = 0.150$ obtained by $1/d$ expansion (Fisher and Gaunt 1964, Balian *et al* 1975).

The exponents y_T and y_H are generally less accurate than the critical couplings in our simple approximation. We remark that our scheme is not designed to yield accurate exponents for all d, because our length rescaling is anisotropic above $d = 1$; moreover, the hyperscaling condition which is involved in the determination of y_H breaks down above $d = 4$. However, for $d \leqslant 4$, our exponents are of about the same quality as those found by Migdal's approximation.

The above discussion has been restricted to ferromagnetic models, but can be generalised straightforwardly to the antiferromagnetic case by making use of boundary conditions which respect the translational symmetry of the staggered order parameter. The possibility of easily incorporating the order parameter symmetry into the boundary conditions is another very interesting and promising feature of the present approach.

Our method can also be applied straightforwardly to quantum systems, where the variety of available renormalisation techniques is definitely smaller. We finish this Letter by discussing an application to d-dimensional spin-$\frac{1}{2}$ Ising systems in a transverse field at zero temperature. The Hamiltonian is now of the form

$$\mathcal{H}(s) = -J \sum_{\langle ij \rangle} s_i^z s_j^z - H \sum_i s_i^z + \Gamma \sum_i s_i^x \tag{13}$$

where s_i^x and s_i^z are Pauli matrices and H and Γ are fields in the z and x directions, respectively. Our approach to the ground state of (13) is analogous to that just described in the classical statistical case. For $d = 1$, for example, we again consider two finite realisations of the system with proper boundary conditions. The smaller system consists of one spin feeling the action of the external fields and interacting through a term $-2Js^z b'$ with two fixed boundary spins ($|b'| \leqslant 1$). Analogously, the bigger system consists of two spins interacting with each other and with the external fields as in (13). The boundary interaction terms are of the form $-Js^z b$ ($|b| \leqslant 1$) for each spin. We compute the ground states $|0\rangle_1$ and $|0\rangle_2$ of the two systems, and the

corresponding magnetisations per spin along the z direction. These must be functions of the dimensionless ratios $x = J/\Gamma$ and $y = H/\Gamma$, and of b' and b, respectively. We then proceed as in the previous cases in order to define a renormalisation mapping for the above dimensionless parameters in the neighbourhood of $y = 0$, using formulae of the same form as (7) and (8). In this way we look for critical fixed points, $x^* = x_c$, and compute the zero-temperature counterparts of the exponents y_T and y_H. The extension to general d can also be obtained easily in this case by including the effect of the dimensionality in the boundary conditions. Our results for x_c are reported in table 2, where they are compared with estimates recently obtained by a variational approach to the same model (Horn 1981). In that approach, the ground state of small systems (clusters) like the ones we are considering, with the same boundary conditions, is determined. Then the parameter b is fixed in a Hartree variational scheme such as to minimise the expectation value of (13) in a state given by a direct product of cluster ground states.

Table 2. x_c values for the Ising model with transverse field. MF 1 and MF 2 indicate the results obtained by the variational method with one- and two-spin clusters, respectively (Horn 1981).

d	1	2	3	4
MF 1	0.500	0.250	0.167	0.125
MF 2	0.585	0.260	0.169	0.126
Our method	0.783	0.300	0.187	0.136
	1[a]	0.327[b]	0.199[c]	0.144[c]

[a] Pfeuty (1970).
[b] Pfeuty and Elliott (1971).
[c] Kogut and Sinclair (1981).

Table 2 shows clearly that our recipe is also very efficient in the quantum case and significantly improves the results over those obtained by mean-field-like calculations of the same complexity. For $d = 1$ we obtain the exponents $y_T = 0.68$ and $y_H = 1.50$ (the exact ones are $y_T = 1$ and $y_H = 1.875$). These values and that of K_c are comparable to $y_T = 0.68$, $y_H = 1.73$ and $K_c = 1.27$ which are obtained using a more standard renormalisation group calculation (Jullien *et al* 1978, Jullien 1981) involving two-spin cells. The nice feature of our recursions is that, at least for K_c, they also give good qualitative results for $d = 3$ and 4, whereas the other renormalisation methods (Jullien 1981) are essentially not practicable above $d = 2$.

Our approach can readily be applied to many other interesting problems. We have in mind, for example, systems with continuous spin symmetry, both quantum and classical, or with competing interactions. For the latter systems, our choice of boundary conditions should allow the easy determination of critical surfaces.

An extension of our method to describe first-order transitions is also highly desirable. Thereby one could possibly overcome the inadequacy of mean-field approximations, which always predict first-order transitions in Potts systems with $q > 2$.

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